

# Relativistic corrections to the energy spectra of completely confined particles

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## Abstract

An analytical expression for the relativistic corrections to the energy spectra of particles completely confined in an one-dimensional limited length in real space is given, based upon the wave property of particles, the relativistic energy-momentum relation and two mathematical equations.

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The quantum confinement is one of the most fundamental problems in low dimensional physics. The expression for the energy spectra of a non-relativistic particle of mass  $m$  confined in an one-dimensional limited length in real space between  $x = -L/2$  and  $x = L/2$  has been given in almost any standard quantum mechanics textbook as a classical example of solving the one dimensional Schrödinger differential equation with infinite potential barriers and is well known as

$$E_j = \frac{j^2 \hbar^2 \pi^2}{2mL^2}, \quad (1)$$

where  $j$  is a positive integer. This result is widely used in condensed matter physics, as a theoretical basis of many potential applications of low-dimensional quantum confinement devices[1].

However, as the energy of the confined particle increases, the relativistic effect will show up and the equation (1), which was based on the solution of the non-relativistic Schrödinger differential equation, must be modified. As the energy further increases to very large then there could be even creations of new particles. Here we are interested in the energy range of the particle that the relativistic effect could show up but no new particle's creations.

The usual way of obtaining (1) - solving the Schrödinger differential equation with infinite potential barriers - is not easy to extend to the relativistic case straightforwardly[2]. In the following we use a different approach to give the result of equation (1). The corresponding solution with the relativistic effect can be obtained naturally.

We look the problem from a different way: All plane waves

$$\phi(k, x) = \sqrt{\frac{1}{2\pi}} e^{ikx} \quad -\infty < k < +\infty \quad (2)$$

are a complete set  $C$ , from this complete set  $C$  we can always construct a subset of wavefunctions  $IN \subset C$  by requiring that every wavefunction  $\psi_j(x) \in IN$  to be a standing wave inside the confined real space  $-L/2 < x < L/2$  but zero everywhere outside this region. The standing wave of  $j - 1$  nodes is

$$\psi_j(x) = C_j \sin\left(\frac{j\pi}{L}\left(x - \frac{L}{2}\right)\right), \quad \text{if } |x| < \frac{L}{2},$$

$$= 0, \quad \text{if } |x| \geq \frac{L}{2}. \quad (3)$$

That is, we could choose combination coefficients  $c_j(k)$  to get

$$\psi_j(x) = \int c_j(k) \phi(k, x) dk, \quad (4)$$

and to require  $\psi_j(x)$  to satisfy the equation (3).

Of course,

$$c_j(k) = \frac{j\sqrt{\pi L}}{j^2\pi^2 - k^2L^2} (e^{-ik\frac{L}{2}} - (-1)^j e^{ik\frac{L}{2}}) \quad (5)$$

is the normalized Fourier transform of  $\psi_j(x)$ .

The probability that the confined state  $\psi_j(x)$  has wavevector from  $k$  to  $k + dk$  is  $|c_j(k)|^2 dk$ . Concerning  $|c_j(k)|^2$ , there are two mathematical equations[3]

$$\int_{-\infty}^{\infty} \frac{4j^2\pi L}{(j^2\pi^2 - k^2L^2)^2} \cos^2(kL/2) dk = 1 \quad (6)$$

and

$$\int_{-\infty}^{\infty} \frac{4j^2\pi L}{(j^2\pi^2 - k^2L^2)^2} \cos^2(kL/2) k^2 dk = \frac{j^2\pi^2}{L^2} \quad (7)$$

for odd number  $j$  and similar equations but with the sine function instead of the cosine function for even number  $j$ .

If the plane wave  $\phi(k, x)$  corresponds an eigen value  $o(k)$  of an operator  $\mathbf{O}$ , which is a function of  $k$ , then the corresponding expectation values of the operator  $\mathbf{O}$  in the confined state  $\psi_j(x)$  can be obtained as,

$$O_j = \int |c_j(k)|^2 o(k) dk. \quad (8)$$

It may be noticed that so far *only the wave property of particles is used*.

Based upon equations (6)-(8), we can discuss several different cases:

For non-relativistic particles with a mass  $m$ , the operator  $\mathbf{O}$  we are interested is simply the energy operator  $\mathbf{E}$ . The energy momentum relation of free non-relativistic particles is

$$\varepsilon(k) = \frac{\hbar^2 k^2}{2m}, \quad (9)$$

naturally

$$\begin{aligned} E_j &= \int |c_j(k)|^2 \frac{\hbar^2 k^2}{2m} dk \\ &= \frac{j^2 \hbar^2 \pi^2}{2mL^2} \end{aligned} \quad (10)$$

by using equation (6) and (7). This is exactly the same as equation (1).

For particles without mass, we have  $\mathbf{O} = \Omega^2$  and

$$\omega^2(k) = c^2 k^2, \quad (11)$$

therefore

$$E_j = \hbar \Omega_j = \hbar c \frac{j\pi}{L}. \quad (12)$$

For relativistic particles with static mass  $m$ , we have  $\mathbf{O} = \mathbf{E}^2$  and the corresponding dispersion relation for free relativistic particles is

$$\varepsilon^2(k) = m^2 c^4 + \hbar^2 c^2 k^2, \quad (13)$$

therefore we have

$$E_j^2 = m^2 c^4 + j^2 \hbar^2 c^2 \left(\frac{\pi}{L}\right)^2 \quad (14)$$

by using (6) and (7). Or

$$E_j = \sqrt{m^2 c^4 + j^2 \hbar^2 c^2 \left(\frac{\pi}{L}\right)^2}. \quad (15)$$

In the non-relativistic limit the equation (15) return to equation (10), in addition to a static energy term  $mc^2$ . The author is not aware of (14) or (15) having been published before.

The extension of (14) or (15) to the two or three-dimensional confined relativistic particles is straightforward.

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